

Resonant-pulse operations on the buried donor charge qubits in semiconductors

L. A. Openov

Moscow Engineering Physics Institute (State University), 115409 Moscow, Russia

A new scheme is proposed for rotations of a double-donor charge qubit whose logical states are defined by the two lowest energy states of a single electron localized around one or another donor. It is shown that making use of the microwave pulses tuned to the resonance with an auxiliary excited molecular level allows for implementation of various one-qubit operations in very short times. Decoherence effects are analyzed by the example of the $P_2^+:\text{Si}$ system and shown to be weak enough for experimental realization of this scheme being possible.

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Semiconductor-based devices seem to be very promising for a scalable quantum computing technology [1]. The qubits can be encoded, e. g., in the nuclear or electron spin states [2, 3]. Although the relatively long coherence times make the spin-based qubits good candidates for quantum computation, the single-spin measurement still remains a significant challenge [3, 4]. The charged-based qubits in semiconductors are currently discussed as well, their logical states being encoded in the orbital degrees of freedom of an electron occupying the quantum-dot structure [5, 6, 7, 8]. Coherent oscillations of the double-dot qubit have been observed [8], and the readout schemes have been proposed [9]. In spite of the fact that decoherence of the charge-based qubits [10] is much stronger than of their spin-based counterparts, the charge-based qubits are nevertheless believed to be realizable at the present technological level due to their short operation times.

In view of the technical difficulties concerning manufacturing of the quantum dots with predetermined characteristics, it may appear more reasonable to make use of natural atoms (instead of "artificial" ones) as the localization centers for the electrons carrying qubits. Recent advances in atomically precise placement of single dopants in semiconductors [11, 12] make possible the construction of solid-state atomic qubits. Hollenberg *et al.* proposed a two-atom scheme where the charge qubit consists of two dopant atoms beneath the semiconductor surface [12, 13]. One of the donors is singly ionized, and

the logical states are formed by the lowest two energy states of the remaining valence electron localized at the left or the right donor, $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$, see Fig. 1. Initialization and readout of the qubit are facilitated by a single electron transistor. The surface electrodes are used to control the qubit through the adiabatic variations of the donor potentials.

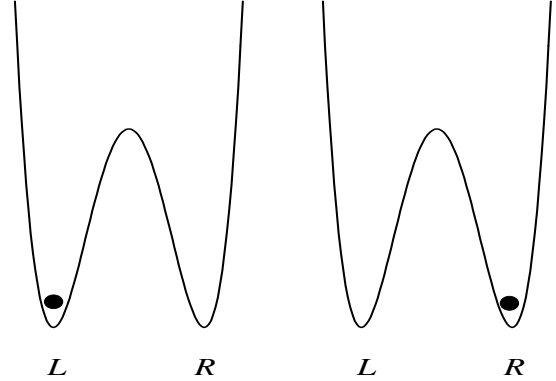


FIG. 1: The logical states $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$ of the buried donor charge qubit.

Here we propose an alternative scheme for rotations of the buried donor charge qubit. Instead of applying biases to the surface gates, the qubit is driven by two microwave pulses tuned to the resonances between the localized states $|L\rangle$, $|R\rangle$ and one of the excited molecular states delocalized over the double-donor structure. We present the analytical solution for the three-level model of the unitary electron evolution and show that, depending on the specific values of frequencies, phases, amplitudes, and durations of the pulses, various one-qubit operations can be implemented in times as short as ~ 1 ps, i. e., more than one order of magnitude shorter than in the original proposal [12, 13]. At such times, decoherence is sufficiently weak, making it possible at least to investigate the small-scale devices and thus to demonstrate the experimental feasibility of the scheme.

We consider a singly ionized pair of dopant atoms in a semiconductor host by the example of the $P_2^+:\text{Si}$ system. The Hamiltonian of the remaining valence electron is

$$\hat{H}_0 = \sum_{n=1} E_n |\chi_n\rangle \langle \chi_n|, \quad (1)$$

where E_n and $|\chi_n\rangle$ are, respectively, the one-electron eigenenergies and eigenstates of the diatomic ion. In order to avoid the sophisticated numerical calculations [14], we ignore the conduction-band anisotropy, the inter-valley terms, the surface effects, etc., and make use of a simple effective mass approximation that is commonly used for the semi-quantitative considerations [15, 16]. Then, in the case that the two donors are equivalent, the problem reduces to that for the hydrogen-like molecular ion with the effective Bohr radius $a_B^* \approx 3$ nm and

the effective Hartree unit of energy $E^* = e^2/\varepsilon a_B^* \approx 40$ meV, where $\varepsilon \approx 12$ is the dielectric constant for silicon. The lowest states $|\chi_1\rangle$ and $|\chi_2\rangle$ are the molecular states $1s\sigma_g$ and $2p\sigma_u$, whose wave functions are, respectively, symmetric and antisymmetric about the midpoint of the line joining the two donors. At large donor separation, $R \gg a_B^*$, one has $E_1 \approx E_2 \approx -E^*/2$, while the difference $\Delta E_{21} = E_2 - E_1$ is exponentially small [17], $\Delta E_{21}/E^* = 4xe^{-x-1}[1 + O(1/x)]$, where $x = R/a_B^*$. The excited state $|\chi_3\rangle$ with the energy $E_3 \approx -E^*/8$ is well separated from the states $|\chi_1\rangle$ and $|\chi_2\rangle$ by $\Delta E_{31} \approx \Delta E_{32} \approx 3E^*/8 \approx 15$ meV. At $R/a_B^* > 6$ this is the molecular state $3d\sigma_g$. If the qubit is biased by the static gate voltages, so that the difference $E_R - E_L$ in the energies of the lowest states $|L\rangle$ and $|R\rangle$ localized at different donors greatly exceeds the value of ΔE_{21} , then the states $|L\rangle$ and $|R\rangle$ are good approximations to the lowest eigenstates, and

$$\hat{H}_0 = E_L|L\rangle\langle L| + E_R|R\rangle\langle R| + \sum_{n=3} E_n|\chi_n\rangle\langle\chi_n|. \quad (2)$$

Let the qubit interact with an external electromagnetic field $\mathbf{E}(t) = \mathbf{E}_{01}(t)\cos(\omega_L t) + \mathbf{E}_{02}(t)\cos(\omega_R t + \phi)$ that has two components oscillating at frequencies $\omega_L = (E_3 - E_L)/\hbar$ and $\omega_R = (E_3 - E_R)/\hbar$, where $\mathbf{E}_{01}(t)$ and $\mathbf{E}_{02}(t)$ are the slowly varying envelopes. Then the Hamiltonian becomes

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t). \quad (3)$$

The interaction term $\hat{V}(t)$ is

$$\hat{V}(t) = \mathbf{E}(t) \left[\mathbf{d}_L|\chi_3\rangle\langle L| + \mathbf{d}_R|\chi_3\rangle\langle R| + h.c. \right], \quad (4)$$

where $\mathbf{d}_{L,R} = \langle\chi_3| -e\mathbf{r}|L,R\rangle$ are the electric dipole moments for the transitions $|L,R\rangle \rightleftharpoons |\chi_3\rangle$. In the resonant approximation [18] one has

$$\begin{aligned} \hat{V}(t) &= \frac{1}{2}e^{-i\omega_L t}\lambda_L(t)|\chi_3\rangle\langle L| \\ &+ \frac{1}{2}e^{-i\omega_R t-i\phi}\lambda_R(t)|\chi_3\rangle\langle R| + h.c., \end{aligned} \quad (5)$$

where $\lambda_L(t) = \mathbf{E}_{01}(t)\mathbf{d}_L$ and $\lambda_R(t) = \mathbf{E}_{02}(t)\mathbf{d}_R$. Here we restrict ourselves to the rectangular pulse shapes, so that both $\mathbf{E}_{01}(t)$ and $\mathbf{E}_{02}(t)$ are constant at $0 < t < \tau_{op}$ and zero elsewhere.

It is straightforward to solve the non-stationary Schrödinger equation

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}(t)|\Psi(t)\rangle \quad (6)$$

for the state vector

$$\begin{aligned} |\Psi(t)\rangle &= C_L(t)e^{-iE_L t/\hbar}|L\rangle + C_R(t)e^{-iE_R t/\hbar}|R\rangle \\ &+ C_3(t)e^{-iE_3 t/\hbar}|\chi_3\rangle \end{aligned} \quad (7)$$

and to find the coefficients $C_L(t)$, $C_R(t)$, and $C_3(t)$ provided that $|\Psi(0)\rangle = \alpha|L\rangle + \beta|R\rangle$:

$$\begin{aligned} C_L(t) &= \alpha \left[1 - \frac{2|\lambda_L|^2}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2(\Omega t) \right] \\ &- \beta \frac{2\lambda_L^* \lambda_R e^{-i\phi}}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2(\Omega t), \\ C_R(t) &= -\alpha \frac{2\lambda_L \lambda_R^* e^{i\phi}}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2(\Omega t) \\ &+ \beta \left[1 - \frac{2|\lambda_R|^2}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2(\Omega t) \right], \\ C_3(t) &= -i \frac{\alpha\lambda_L + \beta\lambda_R e^{-i\phi}}{\sqrt{|\lambda_L|^2 + |\lambda_R|^2}} \sin(2\Omega t), \end{aligned} \quad (8)$$

where $\Omega = \sqrt{|\lambda_L|^2 + |\lambda_R|^2}/4\hbar$. From Eq. (8) one can see that at $t = \tau_{op} = \pi k/2\Omega$ (k is a positive integer) the coefficient C_3 vanishes, and the state vector $|\Psi(t)\rangle$ remains in the qubit subspace $\{|L\rangle, |R\rangle\}$. So, the auxiliary excited state $|\chi_3\rangle$ assists the qubit evolution by means of the electron transfer between the states $|L\rangle$ and $|R\rangle$ as the driving field is on but remains unpopulated after the field is off [19].

It follows from Eqs. (7) and (8) that the relative phase shift operation,

$$|\Psi(\tau_{op})\rangle = e^{-iE_L\tau_{op}/\hbar} \left[\alpha|L\rangle + \beta e^{-i(E_R - E_L)\tau_{op}/\hbar} |R\rangle \right], \quad (9)$$

is implemented at $\tau_{op} = \pi k/\Omega$. The quantum NOT operation,

$$|\Psi(\tau_{op})\rangle = \pm e^{-iE_L\tau_{op}/\hbar - i\phi} \left[\beta|L\rangle + \alpha|R\rangle \right], \quad (10)$$

is realized at $\tau_{op} = \pi(2k - 1)/2\Omega$ if $\lambda_L = \mp\lambda_R$ and $\phi = \pi n + (E_R - E_L)\tau_{op}/2\hbar$ (n is an integer). The Hadamard transformation,

$$|\Psi(\tau_{op})\rangle = \pm e^{-iE_L\tau_{op}/\hbar} \left[\frac{\alpha + \beta}{\sqrt{2}}|L\rangle + \frac{\alpha - \beta}{\sqrt{2}}|R\rangle \right], \quad (11)$$

is performed at $\tau_{op} = \pi(2k - 1)/2\Omega$ if $(E_R - E_L)\tau_{op}/\hbar = 2\pi m$ (m is a positive integer). The plus sign in Eq. (11) corresponds to $\phi = 2\pi n$ and $\lambda_L = -\lambda_R(\sqrt{2} - 1)$ or $\phi = \pi(2n + 1)$ and $\lambda_L = \lambda_R(\sqrt{2} - 1)$, and the minus sign corresponds to $\phi = 2\pi n$ and $\lambda_L = \lambda_R(\sqrt{2} + 1)$ or $\phi = \pi(2n + 1)$ and $\lambda_L = -\lambda_R(\sqrt{2} + 1)$.

For the field amplitudes $E_0 \sim 1$ V/cm, the operation time is $\tau_{op} \sim 1/\Omega \sim \hbar/|\lambda_{L,R}| \sim \hbar/ea_B^*E_0 \sim 1$ ns. Increase in the pulse intensity will cause the value of τ_{op} to decrease down to the picosecond time scale, so that the value of τ_{op} can be made much shorter than in the case that the qubit is manipulated by adiabatically varying the potentials of the surface gates [13]. Note that the energies E_L and E_R should be sufficiently different

from each other, $E_R - E_L \sim 1$ meV, in order the qubit rotations could be implemented in times $\tau_{op} \sim 1$ ps.

The uncontrolled interaction of the quantum system with its environment leads to entanglement between the states of the system and the environmental degrees of freedom. This disturbs the unitary evolution of the system and results in the loss of coherence. There are various sources of decoherence in solids. For the buried donor charge qubit decoherence due to the phonon emission/absorption processes was studied in Refs. [13, 15] and found to be much weaker than decoherence due to both Nyquist-Johnson voltage fluctuations in the surface electrodes and $1/f$ noise from the background charge fluctuations. Contrary to this statement, here we show that phonons are the main cause for decoherence at short operation times. For simplicity, we consider the qubit at zero temperature and assume isotropic acoustic phonons with the linear dispersion law, $\omega_{\mathbf{q}} = sq$, where s is the speed of sound.

Electron-phonon coupling in confined systems is described by the Hamiltonian [20]

$$\hat{H}_{ep} = \sum_{\mathbf{q}} \lambda(\mathbf{q}) \hat{\rho}(\mathbf{q}) [\hat{b}_{\mathbf{q}}^+ + \hat{b}_{-\mathbf{q}}] , \quad (12)$$

where $\hat{b}_{\mathbf{q}}^+$ and $\hat{b}_{\mathbf{q}}$ are, respectively, the operators of creation and annihilation of a phonon with the wave vector \mathbf{q} , $\hat{\rho}(\mathbf{q}) = \int d\mathbf{r} e^{i\mathbf{q}\mathbf{r}} \hat{\rho}(\mathbf{r})$ is the Fourier transform of the electron density operator $\hat{\rho}(\mathbf{r}) = \sum_{mn} \Psi_m^*(\mathbf{r}) \Psi_n(\mathbf{r}) |m\rangle\langle n|$, and $\lambda(\mathbf{q})$ is the microscopic electron-phonon interaction matrix element that can be expressed in terms of the deformation potential D and the density of the crystal ρ as $\lambda(\mathbf{q}) = qD (\hbar/2\rho\omega_{\mathbf{q}}\Omega)^{1/2}$, with Ω being the normalizing volume.

Since at $R \gg a_B^*$ the overlap $\langle L|R \rangle$ between the orbitals $\langle \mathbf{r}|L, R \rangle = (\pi(a_B^*)^3)^{-1/2} \exp(-|\mathbf{r} - \mathbf{r}_{L,R}|/a_B^*)$, where $\mathbf{r}_{L,R} = \mp(R/2)\mathbf{e}_x$ are the donor coordinates, is negligibly small, the transitions $|L\rangle \rightleftharpoons |R\rangle$ are suppressed, and decoherence of the lowest states $|L, R\rangle$ is entirely due to dephasing processes, so that the diagonal elements of the density matrix remain unchanged, while the off-diagonal elements are [16]

$$\rho_{LR}(t) = \rho_{LR}(0) e^{-B^2(t) + i(E_R - E_L)t/\hbar} , \quad (13)$$

where

$$B^2(t) = \frac{8}{\hbar^2} \sum_{\mathbf{q}} \frac{|g(\mathbf{q})|^2}{\omega_{\mathbf{q}}^2} \sin^2\left(\frac{\omega_{\mathbf{q}} t}{2}\right) , \quad (14)$$

and

$$\begin{aligned} g(\mathbf{q}) &= \frac{\lambda(\mathbf{q})}{2} [\langle L|e^{i\mathbf{q}\mathbf{r}}|L\rangle - \langle R|e^{i\mathbf{q}\mathbf{r}}|R\rangle] \\ &= -i\lambda(\mathbf{q}) \frac{\sin(q_x R/2)}{[1 + (qa_B^*)^2/4]^2} . \end{aligned} \quad (15)$$

At $\tau_{op} > a_B^*/s$ one has

$$B^2(\tau_{op}) = \frac{D^2}{3\pi^2 \rho \hbar s^3 (a_B^*)^2} , \quad (16)$$

so that the spectral function (14) appears to be a material constant, being about $6 \cdot 10^{-3}$ for $P_2^+:\text{Si}$, and the error rate (i. e., the error generated during the operation time) is [16]

$$D(\tau_{op}) = \frac{1}{2} [1 - e^{-B^2(\tau_{op})}] \approx 3 \cdot 10^{-3} . \quad (17)$$

Since the excited level $|\chi_3\rangle$ becomes temporarily populated during the resonant-pulse operations on the $P_2^+:\text{Si}$ qubit, the phonon emission processes $|\chi_3\rangle \rightarrow |L, R\rangle$ also contribute to decoherence at $T = 0$. For the double donor orientation along the x -axis one has $|\chi_3\rangle \approx [|2S\rangle_L - |2P_x\rangle_L + |2S\rangle_R + |2P_x\rangle_R]/2$ at $R \gg a_B^*$ and $E_R - E_L \ll E_3 - E_{L,R}$. Neglecting the exponentially small overlap between the localized atomic-like orbitals $\langle \mathbf{r}|L, R\rangle$, $\langle \mathbf{r}|2S\rangle_{L,R} = (8\pi(a_B^*)^3)^{-1/2} (1 - |\mathbf{r} - \mathbf{r}_{L,R}|/2a_B^*) \exp(-|\mathbf{r} - \mathbf{r}_{L,R}|/2a_B^*)$, and $\langle \mathbf{r}|2P_x\rangle_{L,R} = (32\pi(a_B^*)^5)^{-1/2} (x - x_{L,R}) \exp(-|\mathbf{r} - \mathbf{r}_{L,R}|/2a_B^*)$ centered at different donors, we have

$$\langle \chi_3|e^{i\mathbf{q}\mathbf{r}}|L, R\rangle = 2\sqrt{2} \frac{(qa_B^*)^2 \mp i\frac{3}{2}(q_x a_B^*)}{[\frac{9}{4} + (qa_B^*)^2]^3} e^{\mp i q_x R/2} , \quad (18)$$

so that the relaxation rate at $T = 0$ is [21]

$$\begin{aligned} \Gamma &= \frac{2\pi}{\hbar} \sum_{\mathbf{q}, L, R} |\lambda(\mathbf{q})|^2 |\langle \chi_3|e^{i\mathbf{q}\mathbf{r}}|L, R\rangle|^2 \delta(\hbar\omega_0 - \hbar\omega_{\mathbf{q}}) \\ &\approx \frac{8D^2}{\pi\rho\hbar s^2 (a_B^*)^3} (q_0 a_B^*)^5 \frac{\frac{3}{4} + (q_0 a_B^*)^2}{[\frac{9}{4} + (q_0 a_B^*)^2]^6} , \end{aligned} \quad (19)$$

where $\hbar\omega_0 = \hbar q_0 s = E_3 - E_L \approx E_3 - E_R \approx 3E^*/8$. From Eq. (19) one has $\Gamma \approx 3 \cdot 10^7 \text{ s}^{-1}$ for $P_2^+:\text{Si}$. We see that at $\tau_{op} < 100$ ps the error rate due to the phonon emission processes [16],

$$D(\tau_{op}) = 1 - e^{-\Gamma\tau_{op}} , \quad (20)$$

is lower than the value of $D(\tau_{op})$ due to dephasing. So, the phonon-induced error rate at $T = 0$ and short operation times is $D(\tau_{op}) \approx 3 \cdot 10^{-3}$. At finite temperatures, such that $k_B T > \hbar\omega_0$, where $\hbar\omega_0 = \hbar s/a_B^* \approx 2$ meV for dephasing processes and $\hbar\omega_0 = E_4 - E_3 \approx E_R - E_L \sim 1$ meV for the processes of the phonon absorption by an electron temporarily occupying the excited state, the error rate increases by a factor of $\sim k_B T/\hbar\omega_0$, i. e., changes slightly at $T < 10$ K.

The error rate due to phonons should be compared to the error rates due to other sources of decoherence. The lowest bounds for the decoherence times associated with the Johnson noise from the gates and the environmental charge fluctuations are [12, 13, 15] $\tau \sim 1 \mu\text{s}$ and $\tau \sim$

1 ns, respectively, so that the corresponding error rates $D(\tau_{op}) = 1 - \exp(-\tau_{op}/\tau)$ do not exceed that due to phonons at $\tau_{op} < (1 \div 10)$ ps. Hence, the performance of the buried donor charge qubit appears to be limited primarily by the electron-phonon interaction.

In conclusion, we proposed a scheme for fast rotations of the buried donor charge qubit through an auxiliary-state-assisted electron evolution under the influence of the resonant microwave pulses. This scheme allows for implementation of the one-qubit operations in times as short as $\tau_{op} \sim 1$ ps. By the example of the $P_2^+:\text{Si}$ qubit, we have shown that dephasing due to acoustic phonons is the main source of decoherence at $T < 10$ K and operation times $\tau_{op} = (1 \div 10)$ ps. The error rate is about $3 \cdot 10^{-3}$, i. e., greater than the fault-tolerance threshold for quantum computation [22] but low enough for coherent qubit manipulation being possible, at least in the proof-of-principle experiments on one-qubit devices. The coupling of the double-donor qubits via the Coulomb interaction allows, in principle, to realize the conditional gates. It would be also worthwhile to search for other materials and/or doping elements for the buried donor charge qubits, in order to weaken the decoherence effects. Although we restricted ourselves to rectangular shapes of the resonant pulses, our consideration can be generalized to other pulse shapes

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